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APPROXIMATION OF MULTIFLUID MIXTURE RESPONSE FOR SIMULATION OF SHARP AND DIFFUSE MATERIAL INTERFACES ON AN EULERIAN GRID

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Abstract. Multimaterial Eulerian and Arbitrary Lagragian-Eulerian (ALE) codes usually use volume fractions of materials to track individual components in mixed cells. Material advection usually is calculated either by interface capturing, where a high-order van Leer–like slope reconstruction technique is applied, or interface tracking, where a normal reconstruction technique is applied. The former approach is more appropriate for gas-like substances, and the latter is ideal for solids and liquids, since it does not smear out material interfaces. A wide range of problems involves both diffuse and sharp interfaces between substances and demands a combination of these techniques. It is possible to treat all substances that can diffuse into each other as a single material and only keep mass fractions of the individual components of the mixture. The material response can be determined based on the assumption of pressure and temperature equilibrium between components of the mixture. Unfortunately, it is extremely difficult to solve the corresponding system of equations. In order to avoid these problems one can introduce an effective gamma and employ the ideal gas approximation to calculate mixture response. This method provides reliable results, is able to compute strong shock waves, and deals with complex equations of state. Results from a number of simulations using this scheme are presented.

Keywords: Multimaterial, material interfaces, multiphase, mixture models
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INTRODUCTION: A COMBINED SOLID/LIQUID/GAS PROBLEM

Intense loading of complex structures consisting of solids and fluids (as depicted on Fig.1) presents a formidible challenge for numerical simulation. The traditional approaches, where the solid is simulated by a Lagrangian technique coupled with an Eulerian fluid solver, fails here since the solid undergoes severe deformation. Such problems require either an

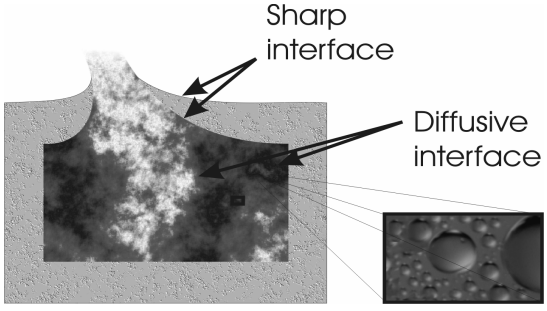

Figure 1. A combined solid/liquid/gas problem with large deformations and diffusive mixing

Eulerian or Arbitrary Lagrange-Eulerian approach. Material interfaces in these cases are usually represented with mixed. In mixed cells, volume fractions of each fluid have to be advected with the material velocity from cell to cell. This process has to be modeled differently for solids, where material interfaces are very sharp, and for fluids, where convective mixing can be a key factor in the flow. Sharp material interfaces are treated with an interface tracking method, where the interface position is reconstructed using volume fraction information from neighboring cells. Diffusive interfaces are implicitly captured, meaning that mass fractions are advected using the single fluid algorithm as a history-dependent parameter.

SHARP MATERIAL INTERFACE TREATMENT

It is of interest to compute large-deformation flows in problems consisting of multiple resolved solids. The algorithm described here treats the propagation of surfaces in space in terms of an equivalent evolution of volume fractions defined by the equation:

$$\frac{\partial f_\alpha}{\partial t} + \nabla \cdot \left(f_\alpha \mathbf{v} \right) = \frac{f_\alpha}{K_\alpha} K \nabla \cdot \mathbf{v}$$

$$1/K = \sum f_\alpha / K_\alpha$$

where f_α and K_α are the volume fraction and bulk modulus of each material α and $\mathbf{v}$ is the velocity in the cell. The approach to modeling multimaterial cells is similar to that in [3]. Specifically, material properties have multiple values in a cell, but the velocity and stress are single valued. In order to use the single-fluid solver it is necessary to define an effective single phase for the mixed cells and to update material volume fractions based on self-consistent cell thermodynamics [3]:

$$1/K = \sum f_\alpha / K_\alpha$$

$$1/G = \sum f_\alpha / G_\alpha$$

$$\sigma_{ii} = 1/K \sum f_\alpha \sigma_{ii\alpha} / K_\alpha$$

$$\sigma_{ij, i \neq j} = 1/G \sum f_\alpha \sigma_{ij\alpha} / G_\alpha$$

where $G_\alpha, \sigma_{ij\alpha}$ are the shear modulus and stress tensor components of material α. Distribution of the velocity gradient amongst each material in the cell is done in a similar way:

$$\mathbf{L}_\alpha = \mathbf{L} G / G_\alpha$$

In order to advect volume fractions we use high order interface reconstruction (interface tracking), which preserves linear interface during translation.

DIFFUSE MATERIAL INTERFACES

In contrast with solid material interfaces, which have to stay sharp in the course of a simulation, gases tend to mix with each other by various mechanisms (molecular diffusion, convective and turbulent motion). The other significant difference is that only the traction vector is continuous on solid material interfaces, while the temperatures are different since each material is deformed adiabatically and thermal flux across the interface is negligible. Temperature in gases, on the other hand, equilibrates much more quickly since the thermal conductivity is higher and, more importantly, other mechanisms related to material mixing are present. Hence pressure and temperature equilibrium between different substances in the gas mixture should be enforced.

Under pressure and temperature equilibrium mass fractions ($m_\alpha = f_\alpha \rho_\alpha / \rho$, where ρ_α is material density) provide enough information to reconstruct the rest of the mixture state variables. The mass fractions can be treated as internal state variables and updated with a simple advection equation

$$\frac{\partial m_\alpha}{\partial t} + \nabla \cdot \left(m_\alpha \mathbf{v} \right) = 0$$

In order to simulate turbulent mixing of components, subgrid scale models are usually employed. Alternatively, a monotonically integrated large eddy simulation (MILES) can be used for turbulence modeling. This idea was introduced in [1] and has been provided with physical rationale by [2]. The idea is that the monotonic integration scheme of discrete finite-volume equations (such as the high-order Godunov scheme we use) produces dissipation due to truncation error comparable to the actual dissipation due to turbulent mixing. So, since we use a MILES-type scheme, turbulent mixing is introduced implicitly by the numerical

approximation and an explicit turbulence model is not required.

In order to calculate pressure and temperature at each time step, we need to solve a computationally expensive nonlinear system of equations to calculate densities and energies of the species:

$$\begin{aligned} &p_\alpha(\rho_\alpha,\varepsilon_\alpha) = p_1(\rho_1,\varepsilon_1) \\ &T_\alpha(\rho_\alpha,\varepsilon_\alpha) = T_1(\rho_1,\varepsilon_1) \\ &\sum \rho_\alpha / m_\alpha = 1 \\ &\sum m_\alpha \varepsilon_\alpha = \varepsilon \end{aligned},$$

where $p_\alpha, T_\alpha, \varepsilon_\alpha$ are pressures, temperatures and specific internal energies of each component. In the two-phase region this system can be singular and non-convergent.

In order to simplify the problem and improve numerical efficiency and robustness, we first consider an ideal gas approximation to calculate properties of the diffusive mixture.

We derive the formulas for an ideal gas, then extend the approach to other gases. The internal energy of multicomponent ideal gas mixture under temperature and pressure equilibrium is:

$$\rho\varepsilon = \rho\sum m_\alpha \varepsilon_\alpha = \rho R T \sum \frac{m_a}{w_\alpha(\gamma_\alpha - 1)},$$

where R is the universal gas constant, w_α is the molecular weight and γ_α is the ratio of specific heats for the gas. Pressure can be calculated by an appropriate weighted sum of partial pressures:

$$p = (1/w)\sum w_\alpha f_\alpha p_\alpha ,$$

where we define an effective molecular weight and effective gamma as follows:

$$w = 1/\sum m_\alpha / w_\alpha$$

$$\frac{1}{w(\gamma-1)} = \sum \frac{m_\alpha}{w_\alpha(\gamma_\alpha - 1)}$$

In order to extend this approach to non-ideal equations of state we need to define an effective gamma, γ_α , for each material. There are many ways to do this; we chose one based on pressure, since it drives hydrodynamic material motion:

$$\gamma_\alpha - 1 = \frac{\hat{p}_\alpha(\rho_\alpha,\varepsilon_\alpha)}{\rho_\alpha\varepsilon_\alpha}$$

This is a relatively slowly varying parameter for a wide range of densities and temperatures for many real materials

Since the mixture is not ideal, we need to make an assumption about the density and energy partition amongst components and calculate the pressure, $\hat{p}$, using a tabulated equation of state. We make the following assumption:

$$\varepsilon_\alpha = \varepsilon$$

$$\rho_\alpha = m_\alpha \rho$$

Then employing the ideal gas relation we calculate:

$$\frac{1}{\gamma-1} = \frac{\rho\varepsilon}{p} = = w\sum \frac{m_i}{w_\alpha(\gamma_\alpha - 1)} = w\sum \frac{m_\alpha^2 \rho\varepsilon}{w_\alpha \hat{p}_\alpha(m_\alpha\rho,\varepsilon)}$$

Finally, the average pressure is:

$$p = \left(w\sum \frac{m_\alpha^2}{w_\alpha \hat{p}_\alpha(m_\alpha\rho,\varepsilon)} \right)^{-1}$$

The initial guess for the specific internal energy (6) can be far from the actual specific internal energy of a given component. Nevertheless, it can yield reasonable results for calculating the overall pressure since it is just used to evaluate an effective gamma for the mixture. We can calculate the zeroth order approximation of cell temperature:

$$T = 1/\sum m_\alpha / \hat{T}_\alpha(m_\alpha\rho,\varepsilon)$$

While this formula will calculate temperatures for individual components $T_\alpha = \hat{T}_\alpha(m_\alpha\rho,\varepsilon)$ incorrectly even for an ideal gas, the average cell temperature will be consistent with the answer for ideal gas:

$$\begin{aligned} T = 1/\sum m_\alpha / T_\alpha = 1/\sum m_\alpha R/(w_\alpha\omega_\alpha\varepsilon) = \\ = \varepsilon/\left(R\sum m_\alpha/(w_\alpha\omega_\alpha)\right) = w\omega\varepsilon/R \end{aligned}$$

In order to improve the estimate of the temperature of each component, however, we would need to have a better energy estimate. Once we have calculated the pressure and γ_α for a given component, we can improve our energy guess for the temperature calculation as follows:

$$\varepsilon_\alpha = w(\gamma-1)\varepsilon/\left(w_\alpha(\gamma_\alpha - 1)\right)$$

In this way, it is possible to construct an iterative procedure to determine component states corresponding to pressure and temperature equilibrium. However, this is (computationally) quite expensive so we have chosen to use a zeroth order estimate.

RESULTS AND DISCUSSION

A problem to test our method of diffusive interface treatment has been simulated. This is a 1D shock tube with initial material states as shown in Fig. 2. These conditions were chosen to be representative of material states in the problems in [4]. Fig. 3 depicts profiles of pressure and temperature after 200 steps. The dashed line represents results where the specific internal energy is assumed to be the same for each mixture component, the solid line represents a simulation where the specific internal energy was redistributed based on calculated effective gammas. Overall, the profiles of pressure and temperature for these approximations are very similar and, given the uncertainties in the other parts of the numerical model, we feel it is appropriate to use the simple zeroth order approximation to calculate the pressures and temperatures of the multicomponent mixture in complex multidimensional simulations. Further applications of proposed technique can be found in the complement paper [4].

Air	Water	Air
T=1eV	T=680K	T=300K
p=4GPa	p=24MPa	p=0.1MPa

Figure 2. Initial conditions for 1D Test of Approximate Pressure and Temperature Calculations

CONCLUSIONS

This paper proposed a simple way to combine sharp and diffusive interfaces in one simulation. Turbulent mixing of multicomponent mixtures is simulated by implicit modeling with a monotonic integration scheme. A non-iterative robust method to calculate mixture properties (pressure and temperature) has been developed

Further work may include an algorithm to dynamically convert material from solid or liquid phase to gas for diffusive mixing based on a multiphase equation of state.

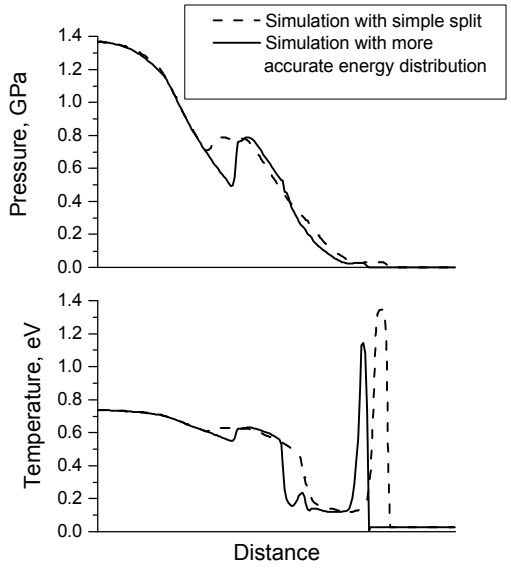

Figure 3. Similation of 1D Test with Approximate Pressure and Temperature Calculations

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